

Pharmacophore Analysis of *Moringa oleifera* Seeds Constituent as Anti-diabetic Properties

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ABSTRACT Pharmacophore modeling approach is a computer-aided drug design (CADD) method which possessed potential as the most promising candidates to focus on the experimental efforts in modern medicinal chemistry. *M. oleifera*, a well known traditional medicine used for many natural therapeutic such as treatment of inflammation, headache and to combat vitamin deficiency. One of the most important properties that found in *M. oleifera* seeds is anti-diabetic which can prevent from rising of blood sugar level in the body. By using ligand-based pharmacophore Modelling approach, four of established diabetic medicined which is (glibenclamide), (Metformin), (Repaglinide) and (nateglinide) from published literature and database (training set) used to generate the pharmacophore modelling using Ligandscout 4.1 computer software along with the seeds constituent (test set) to determines the closest proximity. The selected seeds contituent are (4-(β -D-rhamnopyranosyloxy)benzyl isothiocyanate), (4-(4 β -O-acetyl- α -L-rhamnopyranosyloxy) benzyl isothiocyanate), (4-(α -L-rhamnopyranosyloxy) benzyl glucosinolate a), (niazimicin), (pterygospermin), (quecertain) and (kaempferol). Result shown the best constituent which is 4-(α -L-rhamnopyranosyloxy) benzyl glucosinolate and 4-(4 β -O-acetyl- α -L-rhamnopyranosyloxy) benzyl isothiocyanate show anti diabetic properties.

KEYWORDS: Pharmacophore modelling, *Moringa oleifera*, Ligandbased, Anti-diabetic

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INTRODUCTION

Diabetic is a disease in which blood glucose levels are above normal. Most of the food we eat is turned into glucose, or sugar, for our bodies to use for energy. The pancreas, an organ that lies near the stomach, makes a hormone called insulin to help glucose get into the cells of our bodies. According to the Malaysian Diabetes Assosiation (MDA), compared to 2006 where only 8.6 percent adults in Malaysia had diabetes, the most recent study done in 2011 showed 15.2 percent adults were diabetic. Diabetes was a chronic disease that can be prevented and for those affected, diabetes can be managed to delay or prevent its complications. Diabetes disease were divided into 2 types which is **type 1** and **type 2** diabetes. Diabetes Mellitus is one of the commonest chronic non-communicable diseases globally (Ibrahim *et al.*, 2010). The **type 1** diabetes known as insulin-dependent diabetes mellitus (IDDM) , usually occurred for about 5% of all diagnosed cases of diabetes. **Type 2** diabetes, which was previously called non-insulin-dependent diabetes mellitus (NIDDM) and mostly for about 90% to 95% of all diagnosed cases of diabetes.

The basic of antidiabetic medications is stimulating insulin production from the pancreas or increasing the sensitivity of the body cells to insulin and is commonly used along with insulin (Bibi *et al.*, 2013). Different classes secretagogues known as sulfonylureas and meglitinides. Insulin sensitizers are biguanides, thiazolidinedione and metformin, and important inhibitors are α -glycosidase inhibitors include acarbose and miglitol etc. The side-effects of these medications include extreme hypoglycemia, idiosyncratic liver cell injury, lactic acidosis, digestive discomfort, permanent neurological deficit, headache, dizziness and even death. The basic challenge in curing diabetes is to maintain blood glucose level close to normal levels. These therapies are used as